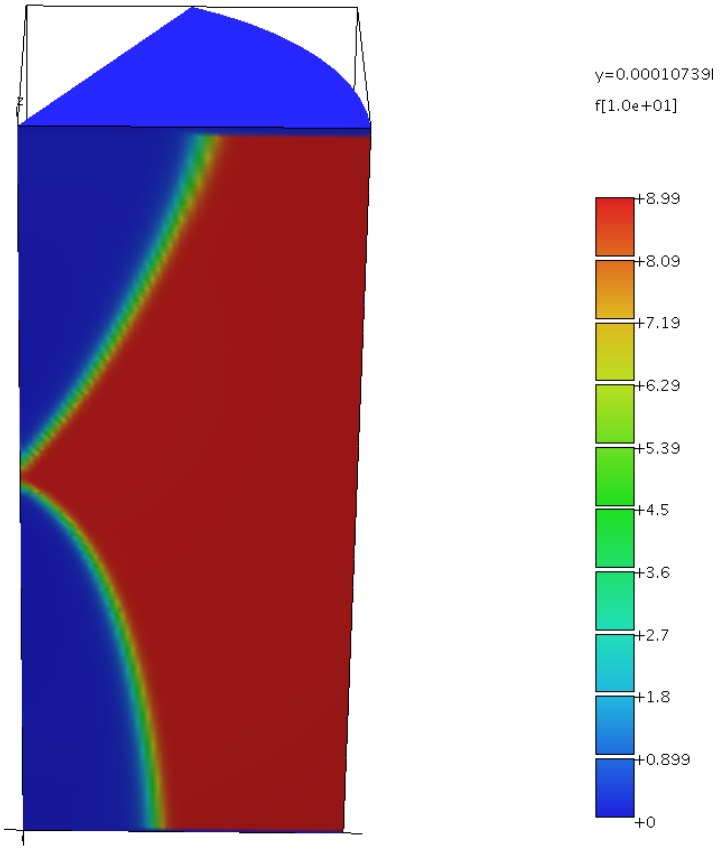
Weierstraß-Institut für Angewandte Analysis und Stochastik

Leibniz Gemeinschaft

K. Gärtner

The van Roosbroeck system, its mathematical properties and their use in device simulation tools



SRH generation 6M pairs, 7.5ns

Outline

- Motivation
- Van Roosbroeck system, analytic/discrete properties
- Sketch of the discretization
- The remaining challenges: grid generation and linear systems
- Example: pin diode, CCD charge handling capacity

Motivation

- Do detector development and device simulation fit well?

- Detector designs span very different requirements:
  sensitivity, speed, spatial, time, energy resolution, noise, ...
  different particles, environments,
  special purpose or mass production
- detectors are not primarily miniaturization driven
- typical are large volumes and geometries from simple to very complicated (large 3d grids are common)
- they can combine detection and amplification
- the classical equations are valid often

- Good chances to increase the common ground!

Van Roosbroeck's Equations

$$-\nabla \cdot \epsilon \nabla w = C - n + p, \tag{1}$$

$$\frac{\partial n}{\partial t} + \nabla \cdot \mu_n n \nabla \phi_n = R, \tag{2}$$

$$\frac{\partial p}{\partial t} - \nabla \cdot \mu_p p \nabla \phi_p = R, \tag{3}$$

$R = r(x,n,p)(n_i^2 - np)$, $r(x,n,p) > 0$, Boltzmann statistics,
w electrostatic potential, ..., in $S \times \Omega$, $S = (0,T)$,
$\Omega \subset I\!R^N$, $2 \leq N \leq 3$, a bounded polyhedral domain,
$\partial\Omega = \Gamma_D \cup \Gamma_N$, Γ_D closed, positive surface measure.
Boundary conditions:
hom. Neumann on insulating parts,
Dirichlet on Ohmic contacts,
and gates: hom./inhom. Neumann ϕ/w
($\partial w/\partial\vec{\nu} + \alpha(w - w_\Gamma) = 0$, $\vec{\nu}$ outer normal vector). Generic situation
$\xi_1 w + \xi_2 \partial w/\partial\nu + \xi_3 = 0$, with ξ_i defined on $\Gamma = \partial\Omega$, $\xi_1(x,w,\dots) \geq 0$,
$\xi_2(x,w,\dots) > 0$.

Introductory remarks

History:

- Van Roosbroeck 1950 (Nernst-Planck equations ...)
- first simulations: Scharfetter and Gummel 1969 (Allen and Southwell 1955)
- Mock's book 1983 made the problem popular (Gajewski and Gröger, Jerome, Markowich,... analytic results)
- 2d simulations in the early 80s (Bank, Rose and Fichtner, Selberherr, ...)
- Missing was a discrete existence theory.

One goal of the talk:
it is essential to carry over qualitative properties of the analytic problem to properly chosen discretizations.

Related functionals

(w^*, n^*, p^*): thermal equilibrium solution of

$$-\nabla \cdot \epsilon \nabla w^* = f + e^{-w^*} - e^{w^*} \text{ in } \Omega,$$

$w^* = w_D^*$ on Γ_D, $\vec{n} \cdot \nabla w^* + \alpha(w^* - w_\Gamma) = 0$ on Γ_{gate}, $n^* = e^{w^*}$, $p^* = e^{-w^*}$.

Free energy:

$$F(w,n,p) = \int [n(\ln \frac{n}{n^*} - 1) + n^* + p(\ln \frac{p}{p^*} - 1) + p^*] \, d\Omega + \frac{1}{2} |\!|\!| w - w^* |\!|\!|^2,$$

with $|\!|\!| h |\!|\!|^2 = \int \epsilon |\nabla h|^2 \, d\Omega + \int \alpha h^2 \, d\Gamma$.

Dissipation rate:

$$d(w,n,p) = \int [n\mu_n |\nabla \phi_n|^2 + p\mu_p |\nabla \phi_p|^2 + r(x,n,p)(np-1)\ln(np)] \, d\Omega \geq 0.$$

Basic qualitative analytic results

1) thermodynamic equilibrium boundary conditions:
the free energy decays for any initial data along trajectories (exponentially) to its equilibrium value,
the thermodynamic equilibrium is unique;

2) existence of bounded steady state solutions (smoothness assumptions on data, models and domains, space dimensions), uniqueness close to equilibrium, i.e., small applied voltages, popular counter example uniqueness: thyristor);

3) 1d unipolar problem: unique, bounded steady state solution.
4) time dependent problems: existence and uniqueness for finite time intervals (avalanche blow up), in special cases global in time (no 'easy' bounds far from steady state, non trivial attractor dimensions);

5) most of the results are valid for Fermi-Dirac statistics, too.

one source of literature:

http://www.wias-berlin.de/main/publications/wias-publ/index.cgi.en and cited one

What's known in the discrete case?

Suppose
– boundary conforming Delaunay grids,
– a finite volume scheme combined with
the classical Scharfetter-Gummel discretization in space and the implicit Euler scheme in time.

For any h (spatial step size) and τ (time step size) holds:

property	analytic	discrete
dissipativity	yes	yes
exponential decay free energy	yes	yes (no rate)
existence of bounded steady state sol.	yes	yes
uniqueness for small applied voltages	yes	yes

What's known in the discrete case?

Byproduct of proofs:
possible averages for $\mu(x, n, p, |\nabla \phi_i|)$, ... preserving these properties.

Other discretizations: smallness conditions!

A few are known explicitly:
Mock's second order scheme, necessary condition for stability:
$|w_i - w_{nn(i)}| < (3 + \sqrt{3})U_T$, $\forall i, nn(i)$, $nn(i)$: next neighbors of i,
$1V \approx 40U_T$, hence 10 nodes per $1V$ applied voltage ...)

Sketch of the discretization

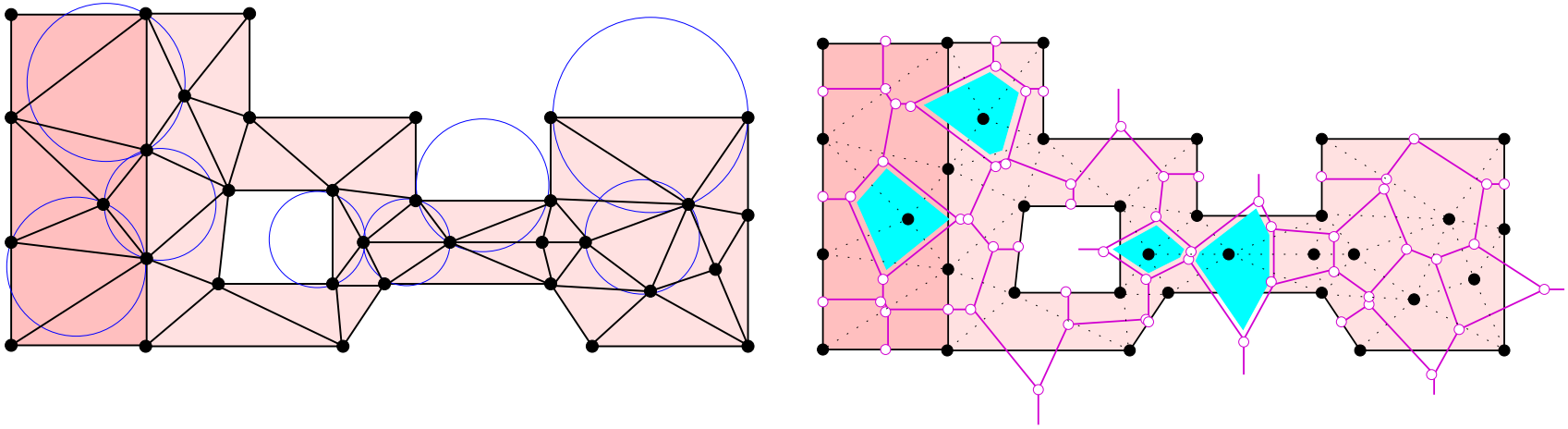
$\mathbf{\Omega} = \cup_i \mathbf{\Omega}_i = \cup_l \mathbf{E}_l^N$, $\mathbf{\Omega}_i$: subdomain, $\mathbf{E}_l^N$: simplex l of dimension N.

Definition 1 *A discretization by simplices $\mathbf{E}_i^N$ is called a Delaunay grid if the balls defined by the $N+1$ vertices of $\mathbf{E}_i^N$ $\forall$ i do not contain any vertex $\mathbf{x}_k$, $\mathbf{x}_k \in \mathbf{E}_j^N$, $\mathbf{x}_k \notin \mathbf{E}_i^N$.*
Let the Delaunay criterion be fulfilled and let all smallest circum balls of all simplices $\mathbf{E}_l^M \in \partial\mathbf{\Omega}_i$, $M = 1, \ldots, N-1$ contain not any vertex $\mathbf{x}_k \in \mathbf{\Omega}_i$, $\mathbf{x}_k \notin \mathbf{E}_l^M$, this mesh is called boundary conforming Delaunay.

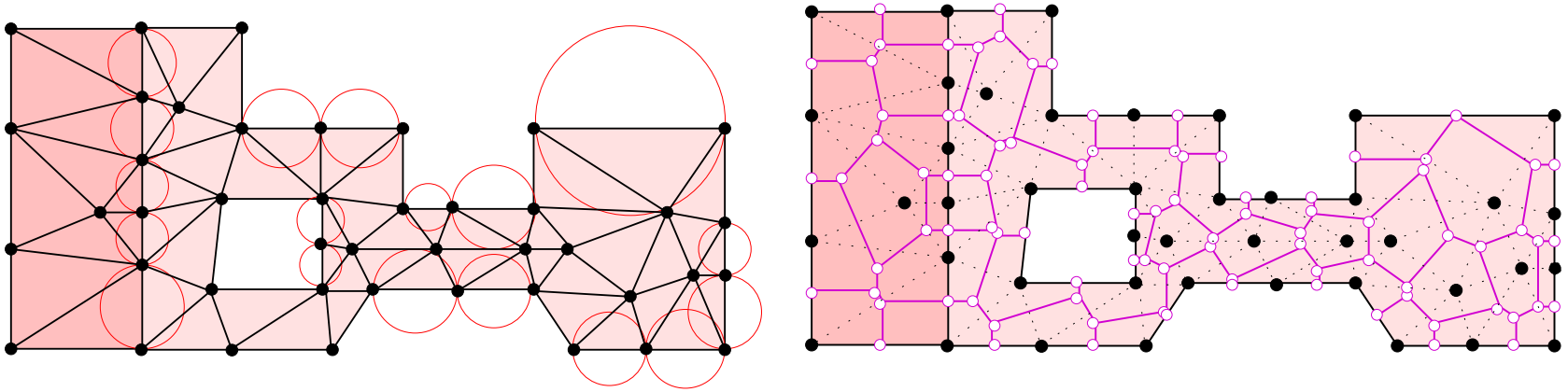
Definition 2 *Let* $V_i = \{\mathbf{x} \in I\!R^N : \|\mathbf{x} - \mathbf{x}_i\| < \|\mathbf{x} - \mathbf{x}_j\|, \forall \text{ vertices } \mathbf{x}_j \in \mathbf{\Omega}\}$
and $\partial V_i = \bar{V}_i \setminus V_i$. V_i is the Voronoi volume of vertex i and ∂V_i is the corresponding Voronoi surface.
The Voronoi volume element V_{ij} of the vertex i with respect to the simplex $\mathbf{E}_j^N$ is the intersection of the simplex $\mathbf{E}_j^N$ and the Voronoi volume V_i of vertex i.
Its surface is denoted $\partial V_{ij} := \partial(V_i \cap \mathbf{E}_j^N)$.

Sketch of the discretization

Delaunay grid:



Boundary conforming Delaunay grid:



Sketch of the discretization

To start with:

$$-\nabla \cdot \epsilon \nabla u = f,$$

$$\begin{aligned}\int_{V_{ij}} -\nabla \cdot \epsilon_l \nabla u \, dV &= -\epsilon_l \int_{\partial V_{ij}} \nabla u \cdot d\mathbf{S}_k = -\epsilon_l \sum_{k(j)} \int_{\partial V_{i,k(j)}} \nabla u \cdot d\mathbf{S}_k + BI_{V_{ij}} \\ &\approx -\epsilon_l \sum_{k} \frac{\partial V_{i,k(j)}}{|\mathbf{e}_{ik(j)}|}(u_k - u_i) + BI_{V_{ij}} = \epsilon_l [\gamma_{k(i)}] \tilde{G}_N \mathbf{u}|_{E_j^N} + BI_{V_{ij}}\end{aligned}$$

where $BI_{V_{ij}}$ denotes boundary integrals in case of boundary conditions; $(u(s)')' = 0$ results in $u' = const$, $u(s_2) - u(s_1) = (s_2 - s_1) * const$.
$\tilde{G}_N$ is a difference matrix, mapping from nodes to edges.

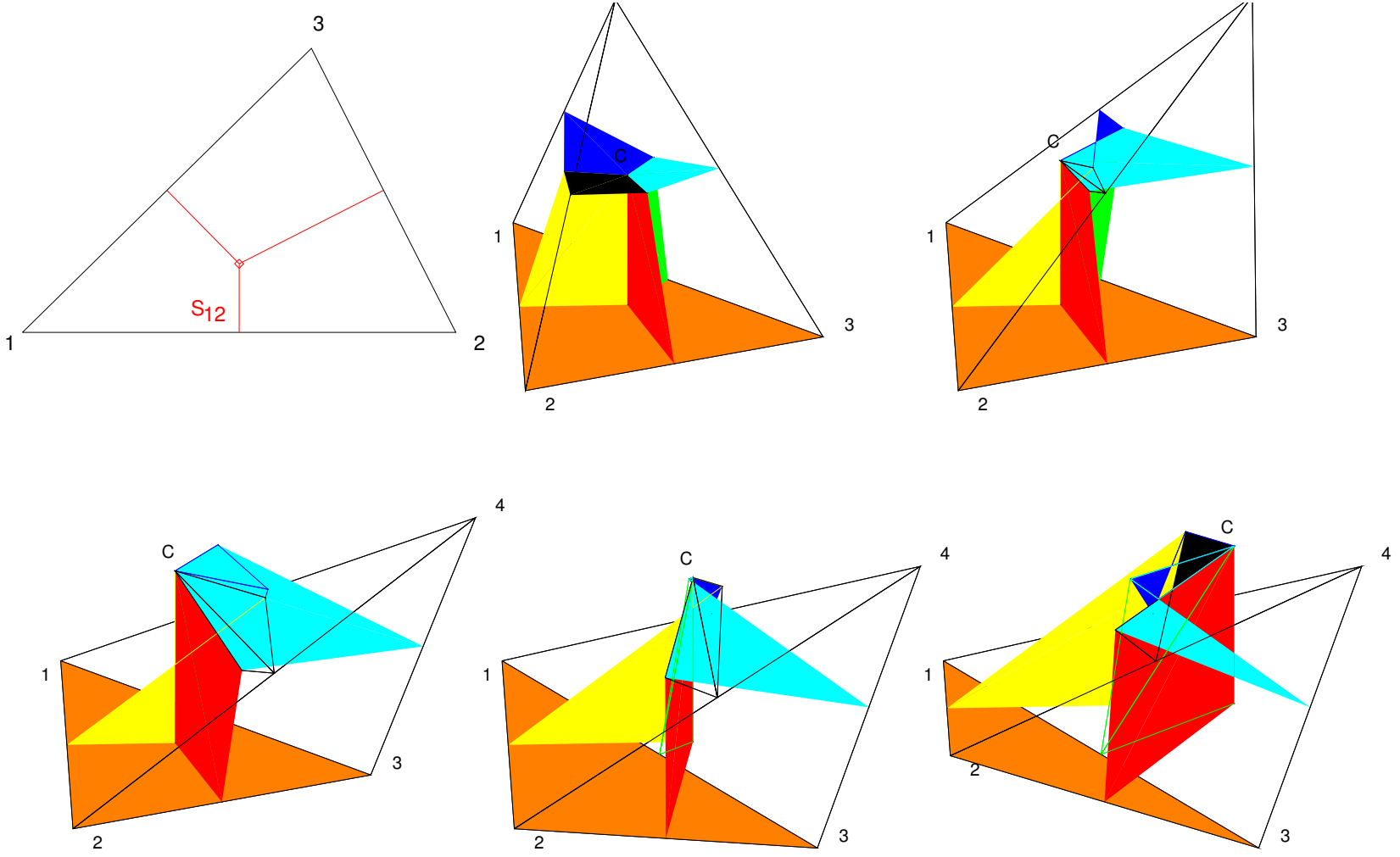
$$(\tilde{G}^T \tilde{G})_{ii} > 0, \quad (\tilde{G}^T \tilde{G})_{i>j} < 0, \text{ and } \mathbf{1}^T \tilde{G}^T = \mathbf{0}^T. \tag{4}$$

$$\gamma_{k(i)} = \frac{\partial V_{i,k(i)}}{|\mathbf{e}_{ik(i)}|}$$

denotes the elements of a diagonal matrix of geometric weights per simplex.

Sketch of the discretization

What is V_{ij}?



Sketch of the discretization

Functions are approximated by

$$\int_{V_{ij}} f dV \approx V_{ij} f(x_i), \quad [V]_i = \sum_j V_{ij},$$

where $[\cdot]$ denotes a diagonal matrix.
Summing over all vertices of the simplex j yields

$$\sum_{V_{ij} \in \mathbf{E}_j^N} \int_{V_{ij}} -\nabla \cdot \epsilon \nabla u \, dV \approx \epsilon \tilde{G}^T [\gamma] \tilde{G} \mathbf{u}|_{E_j^N} + BI.$$

The explicit form of the boundary integrals is given by

$$BI_{V_{ij}} = \sum_{i' \neq i, i' \in \mathbf{E}_j^N} \int_{E_{i'}^{N-1} \cap \partial V_{ij}} -\epsilon \nabla u \cdot d\mathbf{S} \approx \sum_{i' \neq i, i' \in \mathbf{E}_j^N} |E_{i'}^{N-1} \cap \partial V_{ij}| \frac{\epsilon}{\xi_{2_{i'}}} (\xi_{1_{i'}} u_i + \xi_{3_{i'}}),$$

where $E_{i'}^{N-1}$ denotes the $N-1$ dimensional simplex opposite to $i' \in \mathbf{E}_j^N$, $E_{i'}^{N-1} \in \partial\mathbf{\Omega}$, and $BI = \sum_{i \in \mathbf{E}_j^N} BI_{V_{ij}}$.

Sketch of the discretization

A 'weak discrete maximum principle' holds ($\mathbf{u}^+$ pos. part)

$$(\mathbf{u} - u_0)^{+T} \tilde{G}^T [\gamma] \tilde{G} \mathbf{u} > 0,$$

if $\mathbf{u} > u_0$ at least for one $\mathbf{x}_i \in \Omega$, as long as the Voronoi faces related to each edge and subdomain fulfill

$$\sum_{E_j^N \ni \mathbf{e}_{ik}, E_j^N \in \mathbf{\Omega}_l} \partial V_{ik} \geq 0.$$

This is exactly the requirement fulfilled by a 'boundary conforming Delaunay mesh' and has to be preserved for acceptable averages $\bar{\epsilon}_{ij}$ in case of $\epsilon = \epsilon(x, n, p, |\nabla \phi|, ...)$.

Sketch of the discretization

Rewriting the van Roosbroeck system

$$-\nabla \cdot \epsilon \nabla w = C - n + p,$$

$$\frac{\partial n}{\partial t} - \nabla \cdot n_i \mu_n e^{w} \nabla e^{-\phi_n} = R,$$

$$\frac{\partial p}{\partial t} - \nabla \cdot n_i \mu_p e^{-w} \nabla e^{\phi_p} = R,$$

application of the discretization scheme with $(\bar{\mu} e^{w(x)} (e^{-\phi})')' = 0$, $w(x)$ piecewise linear, $u = e^{-\phi_n}$, $v = e^{\phi_p}$ yields
($\mathrm{sh}(s) := \sinh(s)/s$, $b(2s) = e^{-s}/\mathrm{sh}(s) = 2s/(e^{-2s} - 1)$):

$$G^T[\epsilon] G \mathbf{w} = [V] \mathbf{g}(\mathbf{C}, \mathbf{n}, \mathbf{p}), \;\; \mathbf{g} = \mathbf{C} - \mathbf{n} + \mathbf{p}, \;\; \mathbf{n} = [e^{w}]\mathbf{u}, \;\; \mathbf{p} = [e^{-w}]\mathbf{v}, \qquad (5)$$

$$A_{S_n}(\mu_n, \mathbf{w}) \mathbf{e}^{-\phi_n} = G^T[\bar{\mu}_n e^{\bar{w}} / \mathrm{sh}(\tilde{G}\mathbf{w}/2)] G\mathbf{u} = [V][r(\mathbf{x}, \mathbf{n}, \mathbf{p})](\mathbf{1} - [v]\mathbf{u}), \qquad (6)$$

$$A_{S_p}(\mu_p, -\mathbf{w}) \mathbf{e}^{\phi_p} = G^T[\bar{\mu}_p e^{-\bar{w}} / \mathrm{sh}(\tilde{G}\mathbf{w}/2)] G\mathbf{v} = [V][r(\mathbf{x}, \mathbf{n}, \mathbf{p})](\mathbf{1} - [u]\mathbf{v}). \qquad (7)$$

Sketch of the discretization

Theorem 1 *On any connected, boundary conforming Delaunay mesh with n vertices, the problem (5, 6, 7) with positive Dirichlet boundary measure has at least one solution. It fulfills the bounds ($\underline{u} = \underline{v} = e^{-w^+}$, $\overline{u} = \overline{v} = e^{w^+}$, w^+ sufficiently large with $\max(w|_{\Gamma_D}) - \min(w|_{\Gamma_D}) \leq w^+ < \infty$)*

$$\underline{u} \leq \mathbf{u} \leq \overline{u}, \tag{8}$$

$$\underline{v} \leq \mathbf{v} \leq \overline{v}, \tag{9}$$

and the bounds for w

$$\grave{w} := \min(w|_{\Gamma_D}, \check{w}) \leq w_i^0 \leq \max(w|_{\Gamma_D}, \hat{w}) =: \acute{w}, \tag{10}$$

yield finally

$$\underline{w} = \min(w|_{\Gamma_D}, \ln((\check{C} + \sqrt{\check{C}^2 + 4})/2) - w^+) \leq w, \tag{11}$$

$$w \leq \max(w|_{\Gamma_D}, \ln((\hat{C} + \sqrt{\hat{C}^2 + 4})/2) + w^+) = \overline{w}. \tag{12}$$

.

Sketch of the discretization

Used are: monotonicity, the discrete maximum principle, the Gummel map, Brouwer's fixed point theorem.

Dissipativity and uniqueness for small applied voltages follow (details to app. in SIAM SISC).

One knows a lot of related properties of the discrete system:

- transformation by positive diagonal matrices between the different types of variables,
- similarity to symmetric pos. def. (spd) matrices,
- properties of parts of the discrete Jacobian,

Layman's summary: negative densities – never again!

but only up to rounding ...

Practical road map to IV curves

a) Grid generation;

b) Discretization with proven properties;

c) Implicit, dissipative time discretization,
time step control based on free energy, dissipation rate, source integrals ...;

d) Newton's method and implicit damping;

e) solution of the linear systems;

If b), c), d) are solved, a) and e) are the remaining challenges!

Remaining challenges

Any boundary conforming Delaunay grid is a starting point – the goal is:
the best anisotropic (in the Euclidian metric),
adapted boundary conforming Delaunay grid!
This is a research topic in its own.
Constructions for simple cases are possible and used.

Linear systems: due to the huge condition numbers direct and iterative methods are used in combination.
Complexity estimates direct methods (spd case, d space dimension, n unknowns per space dimension, grids of size $N = n^d$):

Operations for	$d = 2$	$d = 3$
Factorization	$N^{\frac{3}{2}}$	N^2
Solution	$Nlog(N)$	$N^{\frac{4}{3}}$

This causes a practical limit at the order of 10^6 nodes, 128GB!

Dream: $\approx 10^7$ nodes, mainly by algorithmic improvements.

Main steps to get things going:

a) construction of a 2d Delaunay grid

b) extension (transl., rotation) to 3d with boundary, material assignment

c) doping profiles (analytic, 1d, 2d DIOS interpolation)

d) description source distribution (MC results), charge integrals

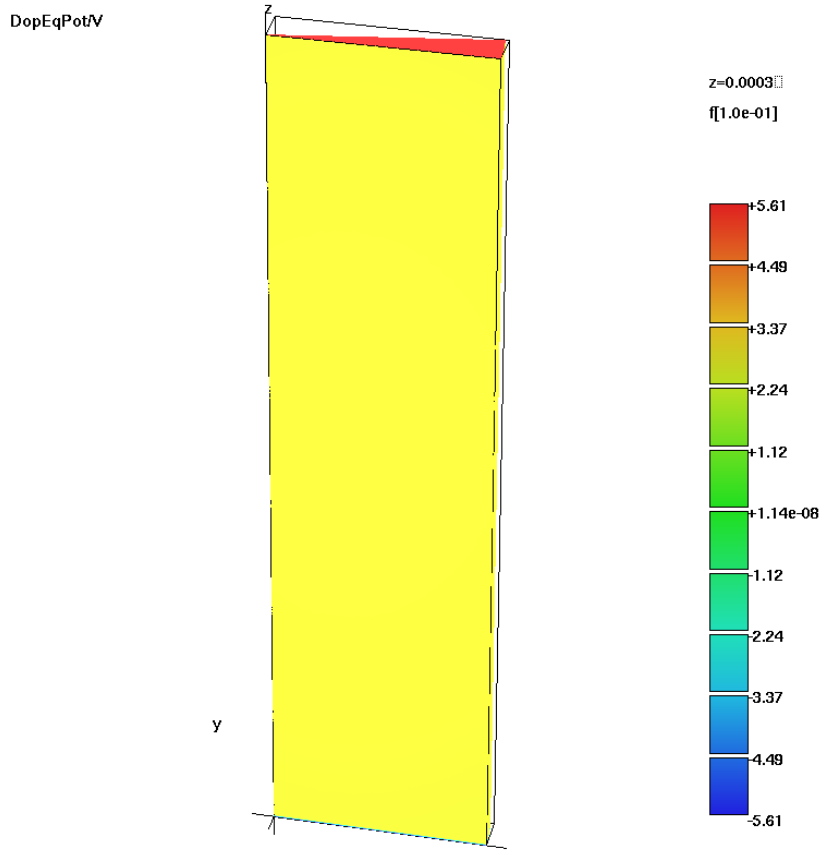
e) material, contact assignment, time functions

...

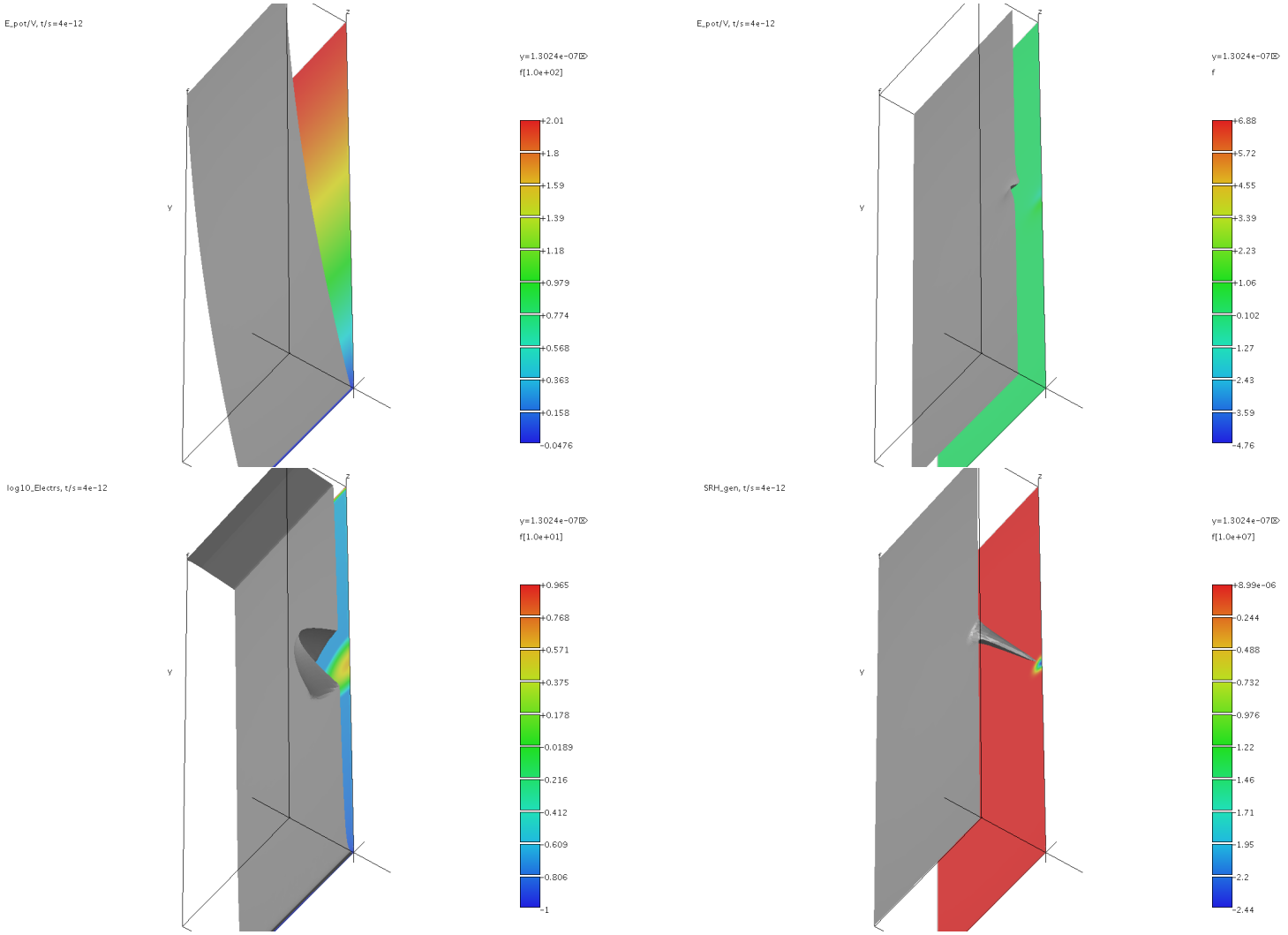
f) IV, I(t), V(t), charge integrals, graphics

pin Diode, 3D

10^o sector,
ToSCA grid in
the $r-z-$ plane,
doping:
top N^+, bottom P^+,
volume $N = 2 \cdot 10^{12}/cm^3$,
top 200V,
depletion 120V,
$R = 75\mu m,\ Z = 300\mu m$,
176 161 nodes,
866 710 tetrahedrons,
1.6M e-h pairs in the
full cylinder

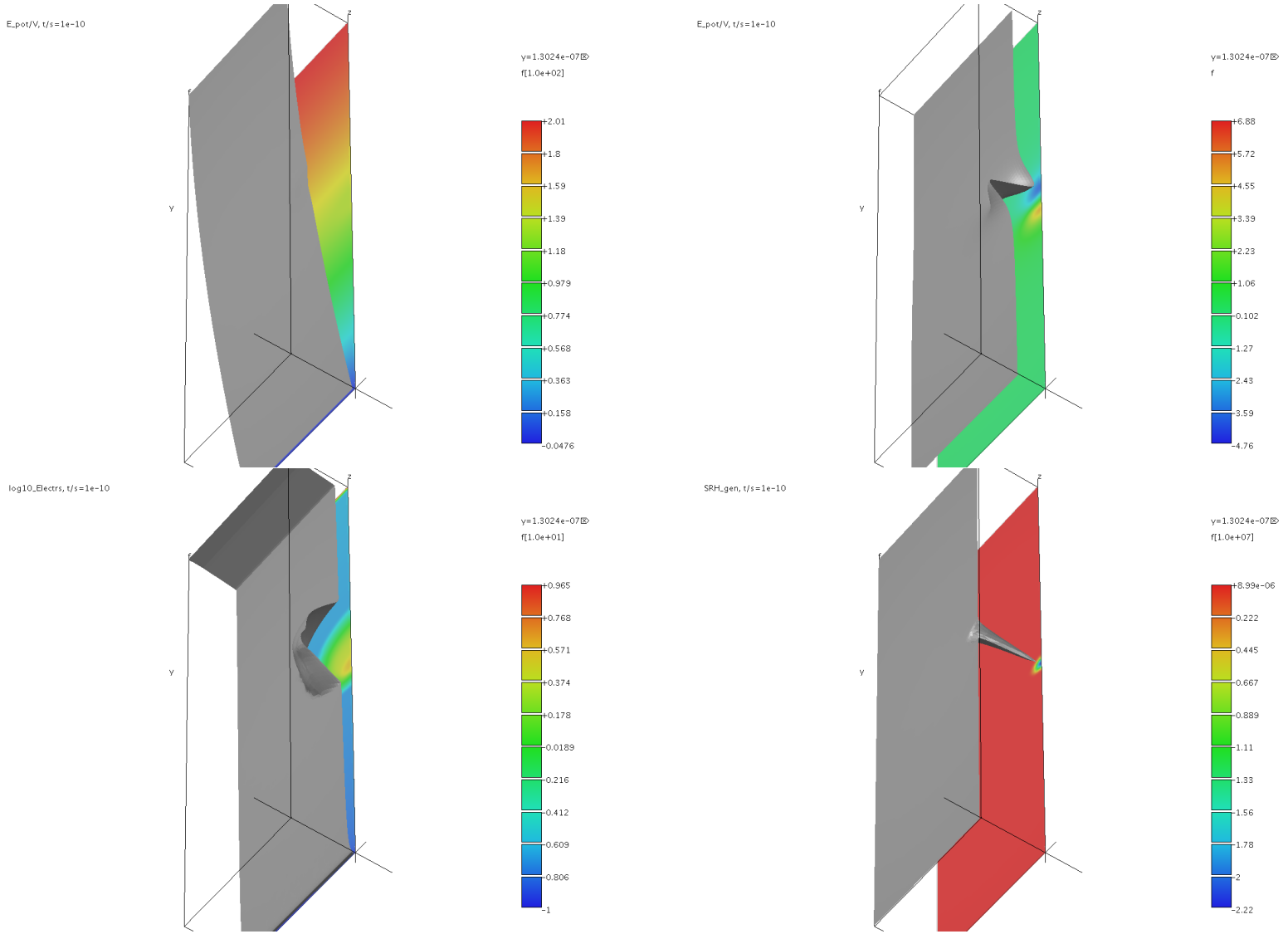


Time scales cloud movement



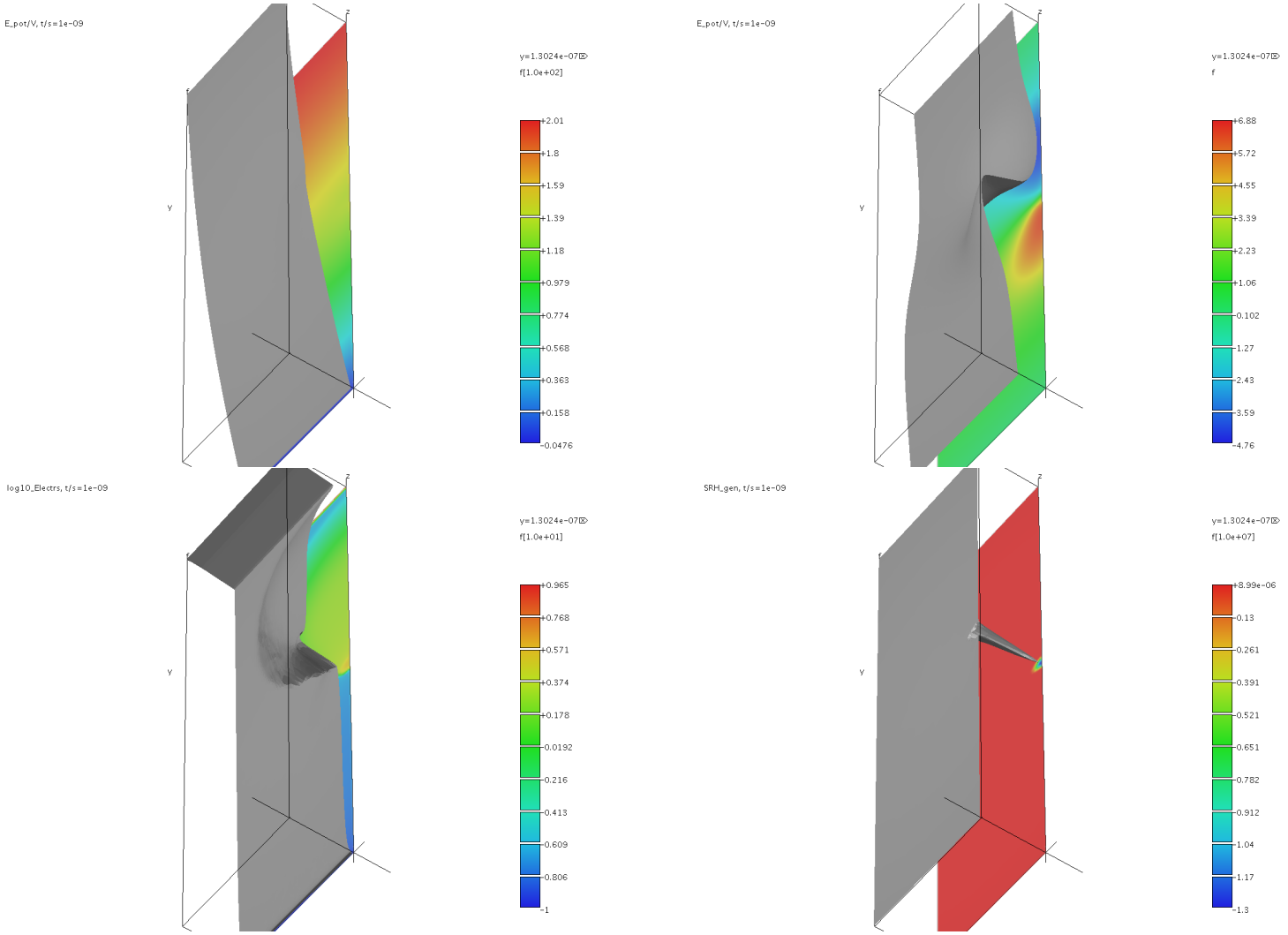
'deposition' time ($4ps$), 'no' changes in the electrostatic pot.

Time scales cloud movement



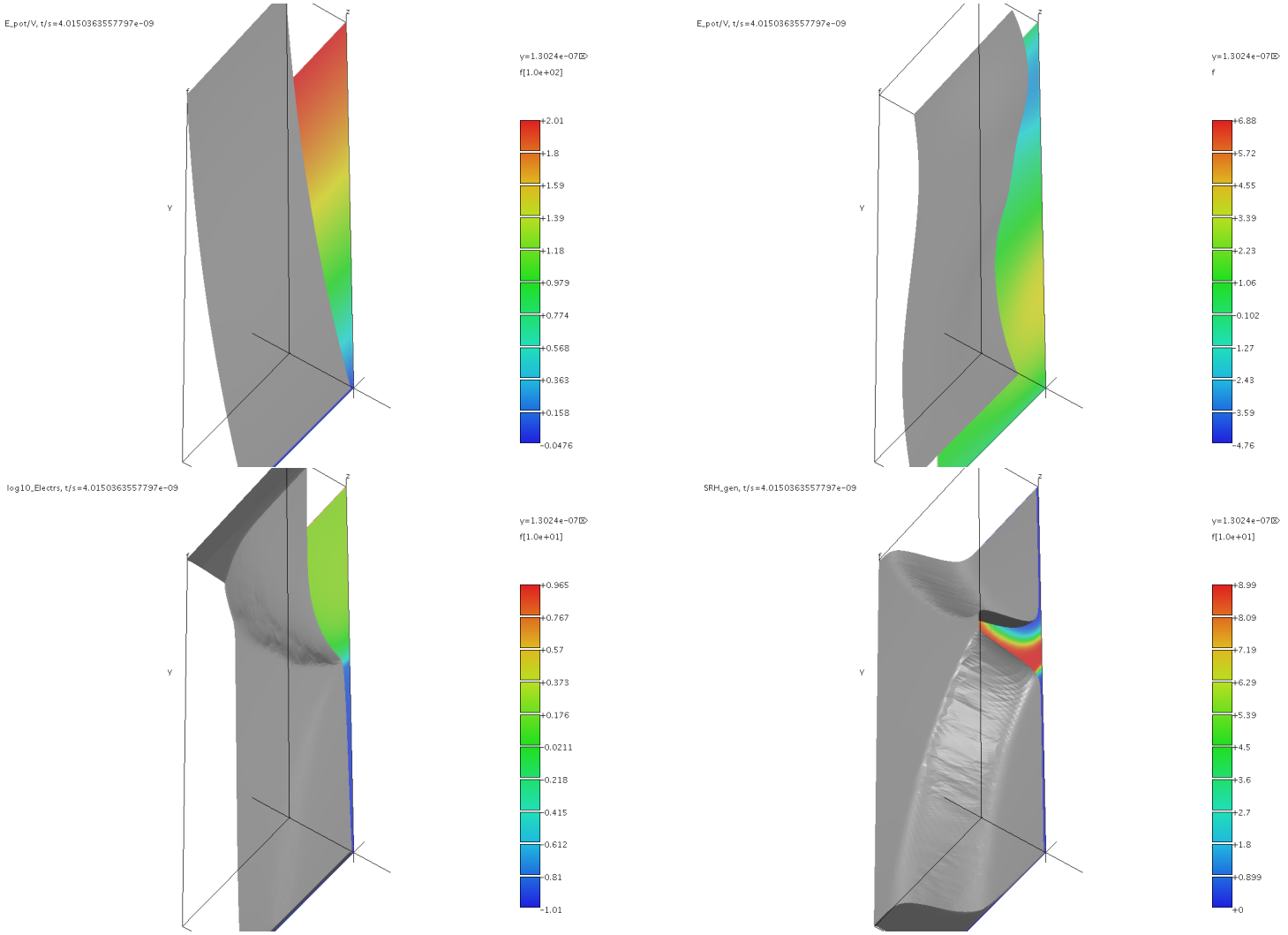
local dd time ($100ps$), 'dipole moment' developed, pot. flattened

Time scales cloud movement



drift time ($1ns$), particle current in the volume

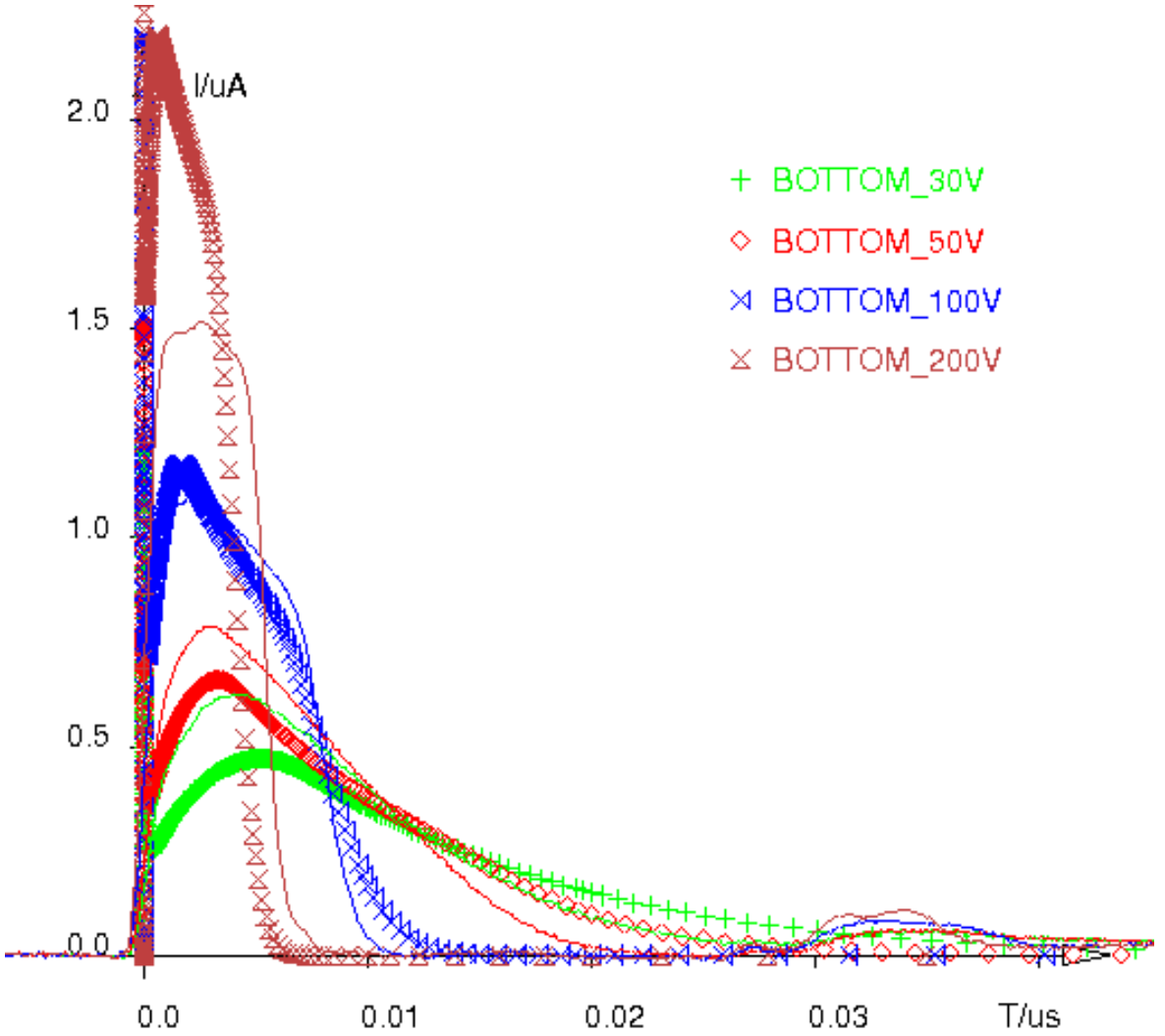
Time scales cloud movement



cloud separation time $0...50ns$, pair number and shape dependent

Charge cloud simulation cooperation

Very first computational results (WIAS) and measurements (lines, Inst. für Experimentalphysik, Uni. Hamburg)



Charge cloud simulation cooperation

Idea and goals:

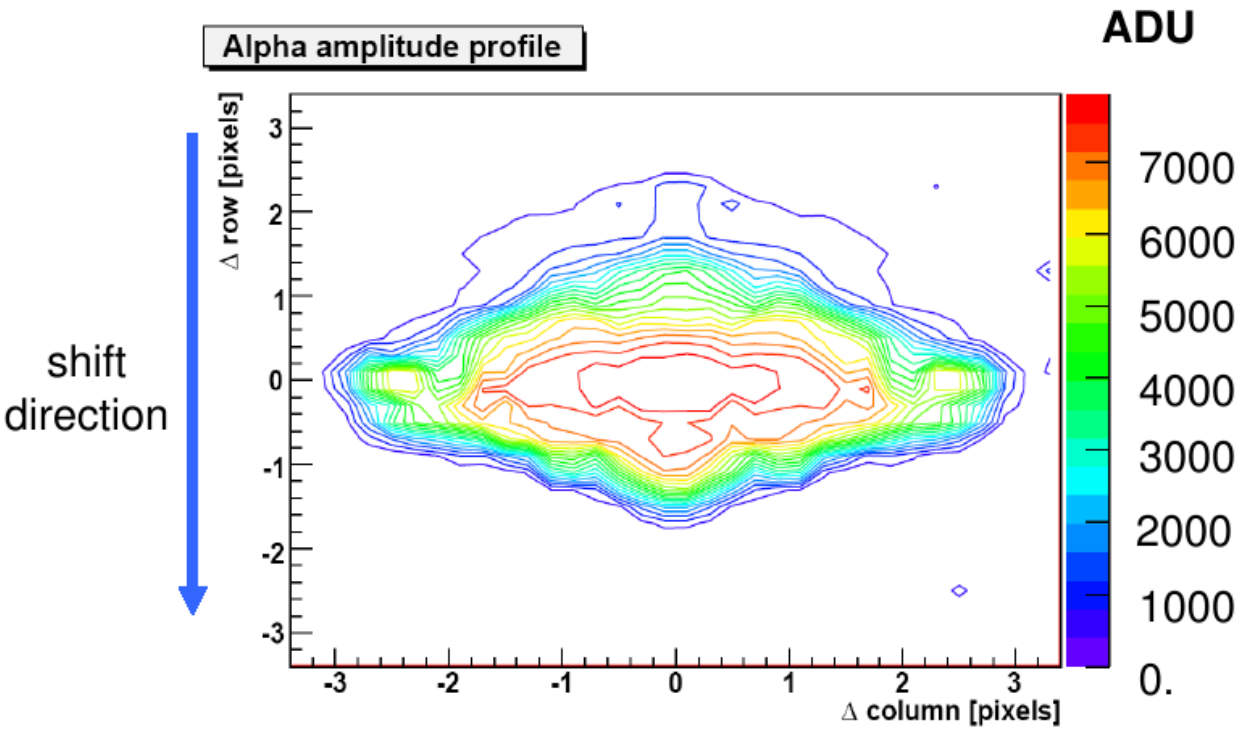
– select a few specific detector design problems with impact (here the huge charge clouds expected at XFEL),
– set up experiments to mimic the future situation (necessary anyway),
– push the simulation limits and compare with the measurements
in a joint effort of detector and applied math people.

This cooperation started including XFEL, HLL Munich, Uni Hamburg, RAL, WIAS a few months ago.

The expected result is:
a simulation code for and influenced by the detector community.

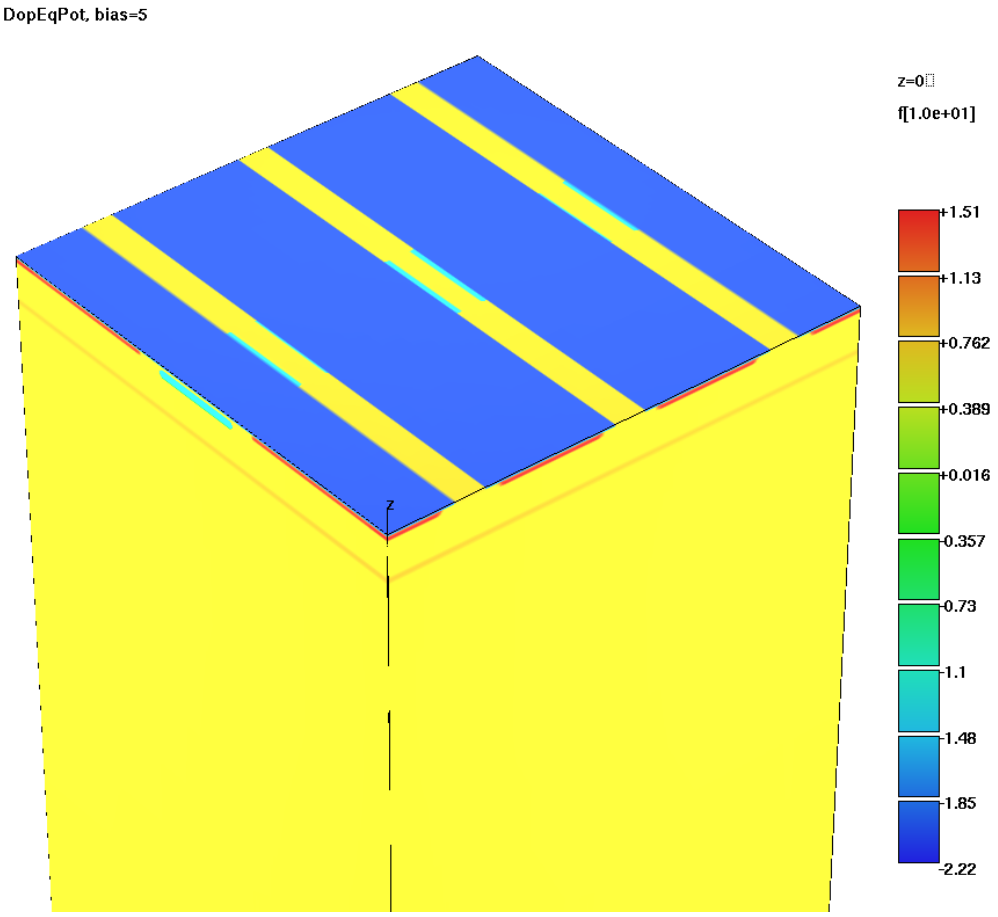
Typical charge spread after an Alpha particle hit (5.5MeV) within a pn-CCD (measurements)

storage pixel size: 75µm x 75µm
frame store pixel size: 75µm x 51µm (relevant for transfer)



Charge spread over 3 pixels in y (shift direction) and 5 pixels in x

Minimal configuration:
total 3 registers
l. blue: channel stop
red storage regions
$X = 75\mu m$, $Y = 75\mu m$,
$Z = 150\mu m$,
958 399 nodes,
5 567 544 tetrahedrons,
BACK -50V, R2=-10V,
R1=R3=R4= -15 / -18V,
MOS1=MOS2=MOS3=5V
Data: HLL Munich

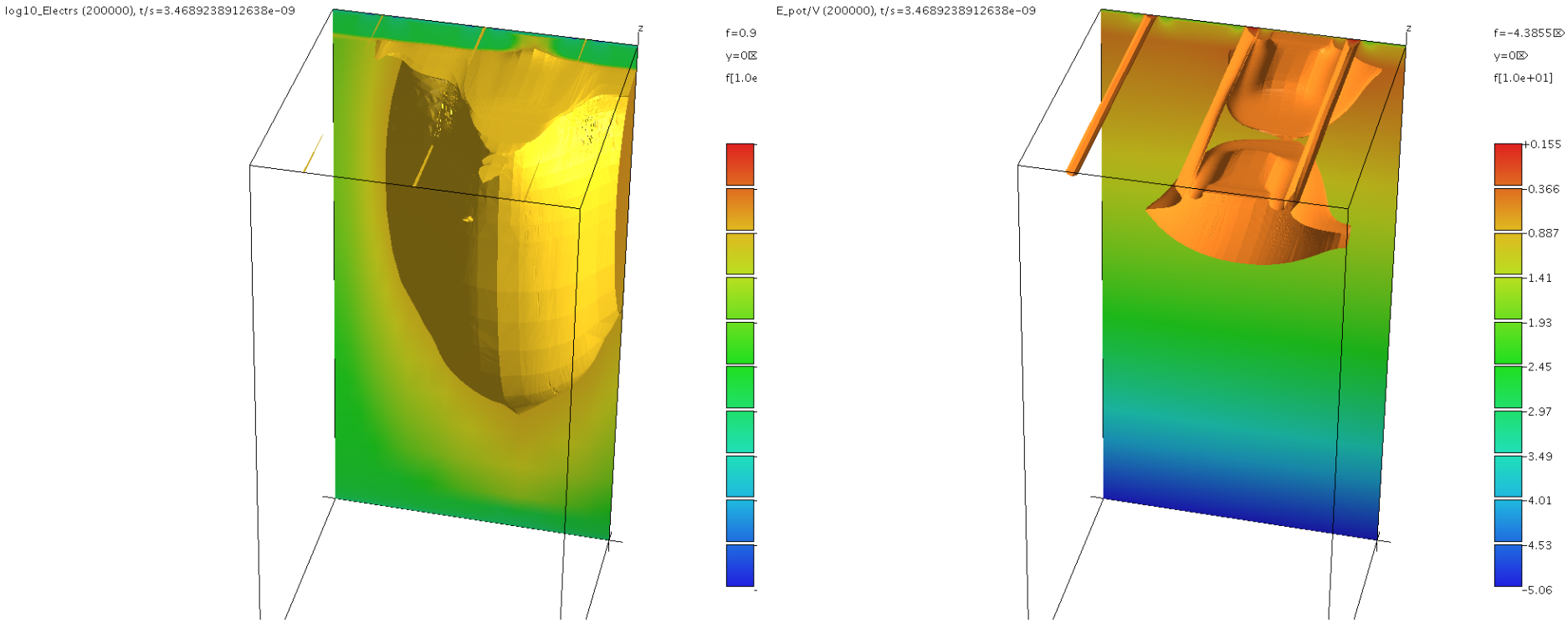


Doping in thermal voltages

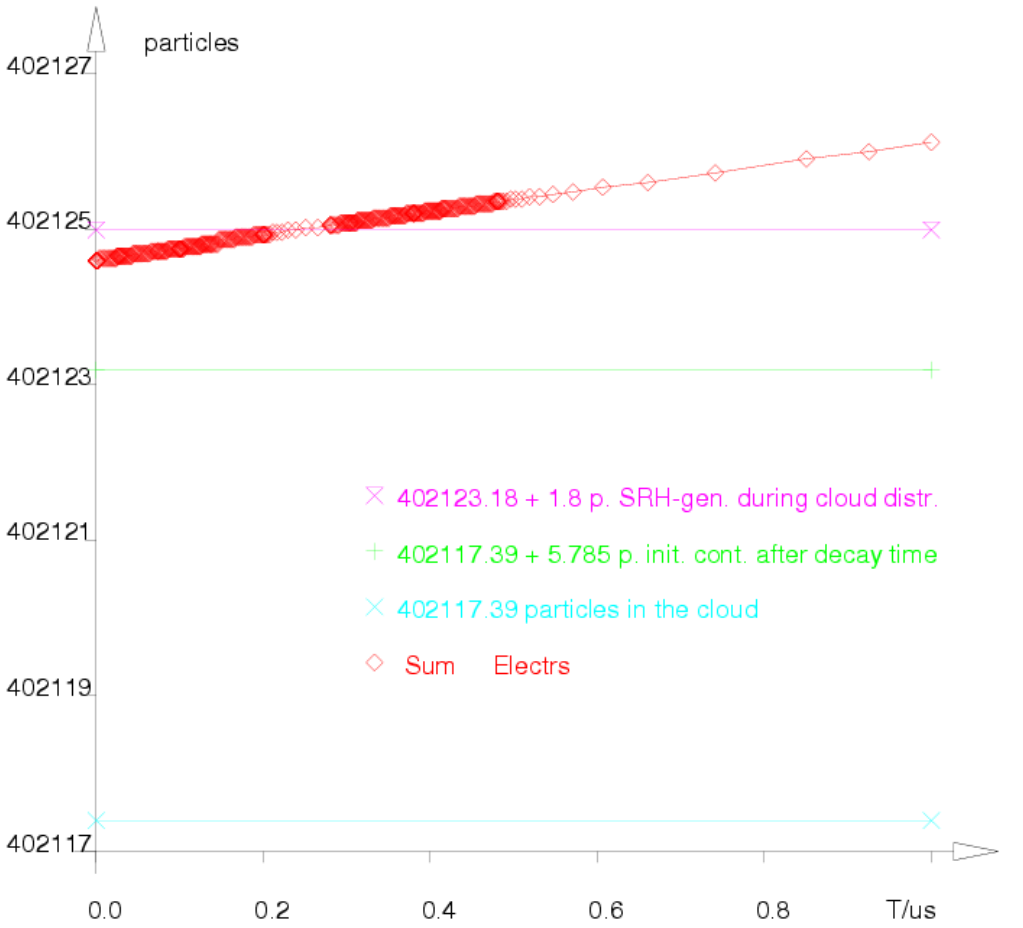
Steps in the computation:

- Depletion,
- reduce n artificially (multiply by 10^{-7}, time integration $0.01as..1ns$), 5.8 electrons are still in the domain;
- start a charge cloud close to BACK beneath R2 and let it distribute;
- shift the electrons: $R2 \to R3 \to R2$;
- check the charge integrals in the lower 99.5% of the domain.

CCD



Overflow of electrons (left), weakest point potential barrier (right, graphics `gltools`)



R1=R4=-18V, MOS1,2,3=5.01V, R2,3(t)=-10V,-18V, BACK=-50V, tau_SRH(5e-3s),

t_shift: 0,100,200,280,380,480ns, 402117.39 electrons, holes started

Total charge balance

Summary

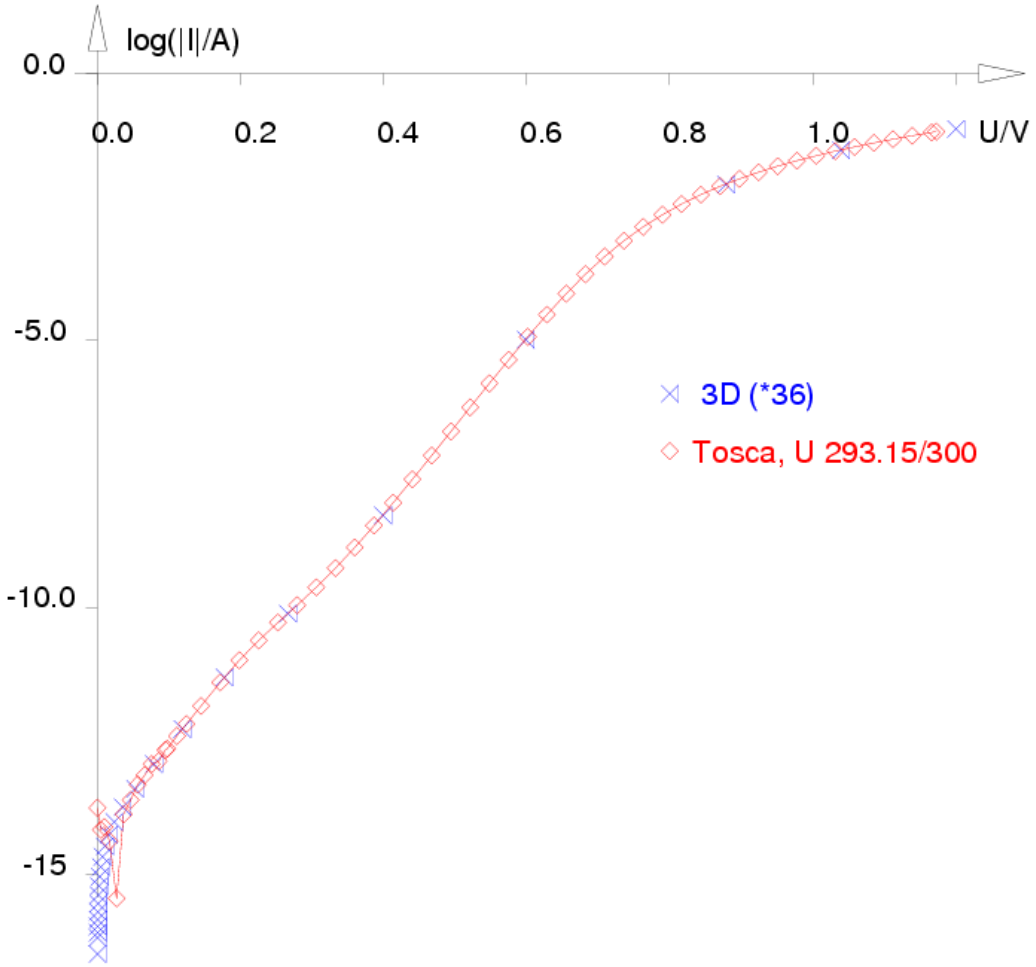
Semiconductor sensor design + advances in device simulation fit nicely.

Thank you for your attention

and HLL Munich for many years of fruitful cooperation.

Van Roosbroeck's Equations

Van Roosbroeck's Equations



3D (293.15K) 10 degree sector versus Tosca (r,z), TOP=0V,

voltage variation at contact BOTTOM

Van Roosbroeck's Equations

The physical meaning of the quantities is :

- $\phi_n = w - \ln n$ - quasi-Fermi potential n,
- $\phi_p = w + \ln p$ - quasi-Fermi potential p,
- $n = e^{w-\phi_n}$ - electron density,
- $p = e^{\phi_p - w}$ - hole density,
- w - electrostatic potential,
- ϵ - dielectric permittivity,
- C - density of impurities,
- R - recombination / generation rate $R = r(x, n, p)(1 - np)$,
- $\mu_{n,p}$ - carrier mobilities $\mu_{n,p} > 0$, Einstein relation.

Scaling of the potentials: U_T, 'thermal voltage', $1V \approx 40U_T$.

Van Roosbroeck's Equations

Rewriting yields:

$$\frac{\partial n}{\partial t} - \nabla \cdot \mu_n(\nabla n - n\nabla w) = R, \tag{13}$$

$$\frac{\partial p}{\partial t} - \nabla \cdot \mu_p(\nabla p + p\nabla w) = R, \tag{14}$$

or

$$\frac{\partial n}{\partial t} - \nabla \cdot \mu_n e^{w} \nabla e^{-\phi_n} = R, \tag{15}$$

$$\frac{\partial p}{\partial t} - \nabla \cdot \mu_p e^{-w} \nabla e^{\phi_p} = R, \tag{16}$$

($e^{-\phi_n}$, e^{ϕ_p} Slotboom variables).